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ABSTRACT

Three improvements to the operational regression procedures used at NOAA/NESDIS to derive total ozone from the TIROS Operational Vertical Sounder (TOVS) measurements are evaluated. An additional predictor, derived from the TOVS measurements, is found to improve the accuracy of the satellite-derived ozone. The substitution for one of the channels used in the regression by another stratospheric channel also improved the accuracy. Finally, the deletion of isothermal cases from the dependent datasets used to derive regression coefficients further improved the accuracy of the ozone determination from the TOVS measurements. The effects of these changes were evaluated with data from the Total Ozone Mapping Spectrometer (TOMS) instrument on Nimbus 7 and the Dobson ozone measurements. Use of these improvements on an independent midwinter set of data from 30° to 65°N resulted in a 4 Dobson Unit (approximately 15%) decrease in the standard deviation of the errors.

1. Introduction

Planet et al. (1984) discussed the derivation of total ozone from the measurements of the TIROS Operational Vertical Sounder (TOVS) flown on the TIROS-N series of NOAA environmental satellites (Schwalb 1978). The technique employed is multiple linear regression of total ozone amounts from Dobson spectrophotometers against measured radiances. A limitation of that approach is the use of a small dependent sample of approximately 20 Dobson stations, for the derivation of the regression coefficients. These stations are located mainly on the North American continent and Western Europe. Large oceanic areas, including nearly all latitudes below 30°S are not represented in the regression coefficients. In the Southern Hemisphere regression coefficients are derived mainly from Northern Hemisphere stations, but shifted six months to account for the seasonal differences. In practice, this means that the TOVS total ozone values in the Southern Hemisphere are influenced by the Northern Hemisphere Dobson values from six months earlier.

To overcome this lack of data and to provide for a more uniform distribution of global total ozone, the ozone values from the Total Ozone Mapping Spectrometer (TOMS), (Heath et al. 1978) are used in this study along with Dobson measurements to develop an improved algorithm. [TOMS data has been reprocessed with improved ozone absorption cross sections (Fleig et al. 1986); the data for this study were obtained before the reprocessing.] The TOMS measurements have been matched in location and time with the radiance measurements from the TOVS. Each TOVS measurement is matched with the closest TOMS observation from the 5° × 5° grid of daily average values. Because the TOMS uses solar radiation, this matched set is restricted to the daylight hours. Lienesch and Pandey (1985) previously used combined TOMS/TOVS datasets to evaluate the procedures for obtaining total ozone in the TOVS processing. They found that the average errors in total ozone could be reduced about 30% by increasing the number of latitude zones from the three used in TOVS processing to eight and selecting more optimal predictors within each zone. These predictors were found to vary with latitude and season and to be different for the Northern and Southern Hemispheres.

In this study we sought improvements to the satellite estimates of TOVS total ozone by considering changes to the regression algorithm. First, a new predictor dependent upon the atmospheric ozone was developed. This predictor is an effective ozone transmittance derived from the TOVS radiances. Second, the measurements in a CO_2 channel sensing in the midstratosphere were substituted as a predictor for the measurements by a channel sensing lower in the stratosphere. Finally, we removed the near-isothermal atmospheres from the dependent datasets used to derive regression coefficients. Only data from winter periods in the 30° to 70°N zone were studied because they contain large

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variations in total ozone and were considered to be appropriate for testing the impact of these changes on the ozone retrieved from the satellite measurements.

2. Approach

The approach used in the current operational retrieval of total ozone from the NOAA spacecraft is a multivariate linear regression. The predictors are the measured radiances in: channel 3 (14.5 μm), sensing CO_2 in the lower stratosphere; channel 8, sensing the surface in an atmospheric window at 11 μm; and channel 9, sensing in the ozone band at 9.7 μm. Crosby (1980) showed that data in channels 8 and 9 are highly correlated because channel 9 senses the radiating surface as well as the atmospheric ozone. The inclusion of channel 8 as one of the predictors effectively compensates for the surface contributions to the channel 9 measurements. Compensation by channel 8 is evident by the fact that the regression coefficients of these channels have opposite signs. The results of retrievals with these three predictors have been discussed by Planet et al. (1984).

The radiance observed by the satellite instruments (Wark and Fleming 1966) can be expressed as

$$R(\nu) = B[\nu, T(p_0)]\tau(\nu, p) + \int_p^0 B[\nu, T(p)][d\tau(\nu, p)/dp]dp \quad (1)$$

where $R(\nu)$ is the spectral radiance, $B[\nu, T(p)]$ the Planck function at wavenumber ν and temperature $T(p)$, p atmospheric pressure, $\tau(\nu, p)$ the transmittance at wavenumber ν between level p and $p = 0$, and p_0 is the surface pressure.

Muller and Cayla (1983) have shown that in the 9.7 μm ozone band, Eq. (1) may be used to give an approximation for $\tau(\nu, p)$,

$$\tau \approx [R_9 - B_9(T_E)]/[B_9(T_0) - B_9(T_E)] \quad (2)$$

where R_9 is the radiance computed from the channel 9 measurements, B_9 the Planck radiance computed at 9.7 μm—the center of the channel 9 spectral band, T_E a mean temperature of the ozone layer, described below, and T_0 is the temperature of the surface.

Physically, τ is an effective ozone transmittance between the satellite and the surface. Equation (2) shows that the effective ozone transmittance can be computed from the channel 9 measurements and from Planck radiances computed at 9.7 μm from the surface temperature and from the temperature of the ozone layer. The surface temperature, T_0, is obtained from the measurements of channel 8, the atmospheric window. The mean temperature of the ozone layer, T_E, is approximated by the brightness temperature in one of the TOVS channels sensing stratospheric temperatures. The appropriate channel was selected empirically by computing an effective ozone transmittance from each of the three TOVS stratospheric channels and then finding which of these is the best predictor.

3. Development

Five TOVS channels have been used in evaluating the effective ozone transmittance as approximated by Eq. (2). The weighting functions of these five channels are shown in Fig. 1. Channels 1, 2 and 3 sense primarily in the stratosphere. Channel 8, sensing in the atmosphere window, measures the surface temperature. The ozone weighting function (channel 9), shown by the dashed curve, peaks near 50 mb, where the ozone is most abundant.

The Planck radiances in Eq. (2) were computed from the TOVS measurements, which are archived as brightness temperatures (Werbowetski 1981). Radiance errors in the stratospheric channels are estimated to be near 2 mW/(m^2 sr cm^{-1}) (channel 1) and 0.25 mW/(m^2 sr cm^{-1}) (channels 2 and 3) (Lauritsen et al. 1979). These errors are equivalent to approximately 2°K for channel 1 and 0.3°K for channels 2 and 3. The measurements from each of these three channels were used for T_E in Eq. (2) to compute three values of effective ozone transmittance for every TOVS observation. These three values were then evaluated as predictors along with the other TOVS infrared channels. The transmittance calculated using channel 2, whose weighting function peaks near 50 mb, was the most highly correlated with the total ozone as measured by the TOMS instrument. Physically, one might expect this result because the channel 2 weighting function

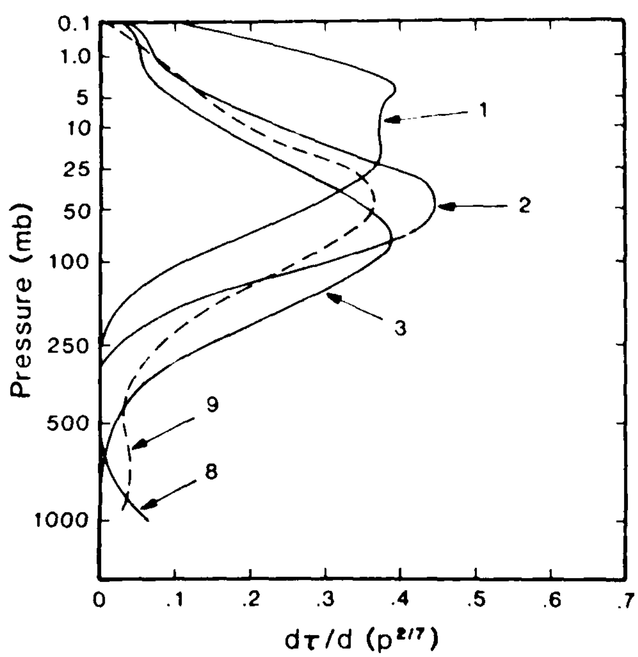

FIG. 1. Weighting functions for the TOVS infrared channels used in the derivation of the effective ozone transmittance (after Planet et al. 1984).

TABLE 1. Correlation coefficients of TOMS total ozone with various predictors for January through March datasets of 1980, 1981 and 1983 over latitudes 40° to 60°N. The wavelengths and species are presented for each channel. The asterisk indicates microwave channels M2 and M4 with frequency specified in GHz. See text for explanation of τ_1, τ_2, and τ_3.

	Channel							Transmittance		
Predictor	1	2	3	8	9	M2	M4	τ_1	τ_2	τ_3
Wavelength (μm)	15.0	14.7	14.5	11.1	9.7	53.8*	58.0*			
Species	CO_2	CO_2	CO_2	Window	O_3	O_2	O_2			
Year	Correlation coefficients									
1980	.50	.71	.69	.37	.44	.56	.70	.67	.76	-.64
1981	.34	.71	.73	.41	.54	.59	.76	.72	.85	-.75
1983	.41	.72	.70	.34	.50	.58	.69	.61	.83	.71

more closely resembles a typical ozone vertical distribution than do those of channels 1 or 3 (see Fig. 1). The maximum concentration of ozone resides in the altitude layer which is contributing most to the channel 2 radiances.

Table 1 shows the central wavelength and the species measured by each channel. This table also contains the correlation coefficients for the radiances in many of the TOVS infrared channels with the TOMS total ozone. Also shown are correlations with radiances in several microwave channels and with the three computed values of ozone transmittance. The data used in the derivation of this table were acquired from the NOAA-6 satellite during January through March 1980, 1981 and 1983. The variable most highly correlated with total ozone is τ_2, the effective ozone transmittance generated in Eq. (2) with T_E from channel 2. Other variables in the table which are highly correlated with the total ozone are τ_1 and τ_3 (the transmittances derived with T_E from channels 1 and 3), the radiances in TOVS channels 2 and 3 and TOVS microwave channel 4. Although the microwave channel M4 correlates with the TOMS total ozone as well as infrared channels 2 and 3, the latter two channels were each found to be better predictors of total ozone when used with the window and ozone channels.

Table 2 shows the reductions in error achieved when the ozone transmittance is added as a predictor of total ozone. This table shows the data from 40° to 60°N for January through March of 1980, 1981 and 1983. Shown are the standard deviations of the residual errors from the computations of the regression coefficients.

TABLE 2. The standard deviation of the residual errors (in Dobson units) derived from various predictors for the TOMS data of January through March of the years 1980, 1981, 1983.

	Residual errors		
Predictors	1980	1981	1983
3, 8, 9	28.9	26.5	26.1
2, 8, 9	27.6	24.6	23.6
2, 8, 9, τ_2	26.3	22.1	21.5

The errors decrease when channels 2, 8 and 9 are used as predictors instead of channels 3, 8 and 9, the predictors used operationally. Additional decreases of several Dobson Units (DU) are achieved with the addition of the ozone transmittance, (τ_2), derived with channel 2 values for T_E in Eq. (2). Comparable improvements are shown for each of the datasets. The standard deviations of the residuals are between 26 and 29 DU when channels 3, 8 and 9 are used as predictors. These values are smaller than those found by Planet et al. (1984). Those authors used Dobson data instead of TOMS in generating regression coefficients for deriving satellite ozone. This table demonstrates that the transmittance value provides additional information about the total ozone. In the following section the impact of this predictor is examined with additional datasets.

4. Application to operations

In the preceding section the TOMS ozone data were used to evaluate potential improvements in the procedures by which the total ozone is derived from the TOVS measurements. However, the operational determination of total ozone from the TOVS instruments on the NOAA satellites is based on regression using the total ozone from ground-based Dobson instruments, not TOMS. The Dobson data are limited spatially and temporally. Therefore, it is important to determine if the techniques derived with the TOMS data are effective when applied to the more restricted Dobson data. Table 3 lists the standard deviations of the errors from the computation of regression coefficients from dependent datasets of Dobson data. The datasets for each year contain the matched TOVS/Dobson observations for January through March. The data are from NOAA 6, 7 and 8. Values are presented for the regressions on radiances in channels 3, 8 and 9 (which are used in the NOAA operational production of total ozone); channels 2, 8, 9 and the effective ozone transmittance, the new predictor set. Results presented in Table 3 were derived from regression coefficients based on data compiled at 12 Dobson stations between 30° and 70°N. It is noteworthy that substituting channel 2 measurements for channel 3 measurements produces

TABLE 3. The standard deviation of the residual errors of TOVS/Dobson regressions for the three-month period of January through March.

Predictors	Satellite	1980	1981	1982	1983	1984
3, 8, 9		35.3	27.1	27.3	32.1	
2, 8, 9	NOAA-6	33.6	26.3	26.5	30.6	
2, 8, 9, τ_2		32.9	23.5	24.8	27.6	
3, 8, 9				28.8	29.3	31.1
2, 8, 9	NOAA-7			27.5	27.3	29.9
2, 8, 9, τ_2				26.5	25.8	29.9
3, 8, 9						31.0
2, 8, 9	NOAA-8					30.8
2, 8, 9, τ_2						30.4

an improvement in every dataset. Adding τ_2 as a predictor produces an additional improvement in nearly every case. The magnitude of the improvement for the NOAA-6 data is similar to that for the TOMS data in Table 2. The standard deviation of the residual errors from the Dobson data (Table 3) are generally larger than those from the TOMS data (Table 2). That result may arise from the fact that the Dobson datasets are constructed from many different ground-based instruments and, consequently, the relationship between the satellite observations of radiance and the total ozone may be somewhat obscured by Dobson instrument differences.

Examination of several of the datasets that went into making Table 3 revealed an occasional satellite observation of an approximately isothermal atmosphere. Isothermal cases are designated as those observations where the stratospheric temperatures measured by channel 2 and the surface temperatures measured by channel 8 differ by 10°C or less. In these instances the ozone transmittance, as derived by Eq. (2), will be unstable because the numerator and denominator are small. The isothermal cases were deleted from the dataset and the statistics derived from the regressions on this reduced dataset were compared to those of the original dataset.

Table 4 shows the standard deviation of the residual errors of the regressions for February 1983 for NOAA-6. The first column, which includes the isothermal cases, shows the results for the regressions based on the Dobson measurements of total ozone. In the next column, the isothermal cases have been deleted. The third and fourth columns are the equivalent values from the regressions performed with the TOMS ozone data over the same period. Deletion of the isothermal cases reduces the residual errors in all cases.

In the preceding paragraphs we have examined the reductions in the residuals from the regressions on the dependent datasets. The question arises as to whether the improved regressions will reduce the errors in calculating total ozone from an independent set of the TOVS measurements. The Dobson-derived coefficients which are used operationally are validated off-line by comparing the retrieved ozone with coincident total ozone measurements obtained from an independent set of Dobson measurements. We also compared the ozone retrieved from the new predictors with those same independent Dobson observations. The results are shown in Table 5 for the data of February 1983. This table shows the impact on the independent dataset when the isothermal cases have been deleted from the dependent datasets used to derive regression coefficients. It should be noted that the independent data shown in Table 5 have not been screened for isothermal cases.

This table summarizes 85 comparisons of satellite ozone with the coincident Dobson ozone from 11 independent Dobson stations between 30° and 65°N. Shown in Table 5 are the results using four sets of coefficients derived from the dependent datasets of February 1983. Column one contains the results from the operational coefficients; in the second column appear

TABLE 4. The standard deviation of the residual errors of TOVS/Dobson and TOVS/TOMS regressions for February 1983.

Predictors	TOVS/Dobson With isothermal cases	TOVS/Dobson Without isothermal cases	TOVS/TOMS With isothermal cases	TOVS/TOMS Without isothermal cases
3, 8, 9	32.1	30.5	26.1	26.0
2, 8, 9	30.6	29.2	23.6	23.3
2, 8, 9, τ_2	27.6	22.8	21.5	20.9

TABLE 5. Comparison of the results from the operational and improved algorithms with the Dobson ozone observations of the independent dataset during February 1983.

	TOVS/Dobson coefficients			TOVS/TOMS coefficients
Predictors	3, 8, 9	3, 8, 9	2, 8, 9, τ_2	2, 8, 9, τ_2
Isothermal cases are:	Retained	Deleted	Deleted	Deleted
Mean Dobson ozone	365.5	365.5	365.5	365.5
Mean satellite ozone	364.8	362.5	358.8	342.2
Mean difference	0.7	−3.0	−6.7	−23.3
Standard deviation	27.9	26.9	23.7	24.4
Corr. coefficient	.86	.86	.89	.89

the results using the operational coefficients with the isothermal cases deleted prior to performing the regressions on the dependent dataset. The third column presents the results for the improved predictors, channels 2, 8, 9 and the transmittance term and with the isothermal cases deleted. The fourth column presents the comparable results based on coefficients derived from the TOMS total ozone measurements where the isothermal observations have also been eliminated prior to computing the regression coefficients. The third and fourth columns utilized the coefficients from regressions having the residual errors shown in columns 2 and 4 of the last row of Table 4.

The first row of Table 5 gives the mean Dobson ozone from the independent dataset of 85 matched Dobson/TOVS observations; thus identical values appear in each column. In the second row the mean values vary because four different sets of coefficients were used in deriving satellite ozone. Row 3 shows a minor change (from −3.0 DU to −6.7 DU) in the mean differences between the satellite-derived ozone when the improved predictors are used and the ozone measured at the Dobson stations. A comparison (not shown) with February 1984 data from NOAA-8 showed an opposite change in the mean differences (from −12 DU to −6 DU) with a reduction in the standard deviation of the errors from 26.6 DU to 24.7 DU. Month-to-month variations of several percent are also observed in the off-line validation of the operationally-derived total ozone with coincident measurements from independent Dobson stations. These biases are not real. They are attributed to month-to-month changes in the composition of the dependent and independent datasets. The variations in the mean differences are less significant than the consistent reductions in the standard deviations achieved with the transmittance term included as a predictor.

The standard deviation of the differences and the correlation coefficient between the satellite and the Dobson ozone are shown on the fourth and fifth rows, respectively. A decrease in the standard deviations of the differences between the satellite-derived ozone and the independent Dobson observations of total ozone is achieved through the use of the new set of predictors. The value decreases from 26.9 to 23.7 DU for the datasets without the isothermal cases. The salient feature in Table 5 is the decrease in the standard deviation from 27.9 for the operational regressions to 23.7 for the new regressions. The slight increase in the correlation coefficients between the satellite-derived ozone and the independent Dobson measures of ozone also indicates that improved values of satellite ozone can be derived from the new set of predictors.

A value of 24.4 DU is shown for the standard deviation of the residual errors when the satellite ozone is derived from the TOMS derived coefficients (column 4) and is tested against the independent Dobson stations. The coefficients from the TOVS/Dobson regressions and from the TOVS/TOMS regressions provide nearly identical improvements except for the large difference in the mean value from the TOVS/TOMS dataset. That value is a direct result of the known bias (Bhartia et al. 1984) existing between the Dobson data and the TOMS data used in this study.

The dataset discussed in the preceding paragraphs is composed of data from January, February, and March 1983. That set was selected for an evaluation of the new procedures because of the relatively large values of the residual errors for the operational regression for that period (see Table 3). Further evaluation of these improvements to the algorithm for deriving total ozone should include periods of relatively low errors that are observed during the other seasons. Prior to implementing these improvements in the operational regressions, an assessment of these algorithm changes over a full year and for other latitude zones will be undertaken. Attention will also focus on regions of high and low ozone where the regression algorithm produces ozone values biased toward the mean.

5. Summary

Total ozone retrieved from the NOAA polar-orbiting spacecraft utilize regressions on measurements in three

channels in the infrared region. The coefficients for these retrievals are compiled from matched TOVS and ground-based Dobson observations. We showed that an additional predictor, an effective ozone transmittance derived from the satellite infrared measurements, was effective in reducing the errors in retrieving total ozone. This technique, originally developed on a dependent sample of matched TOVS and TOMS observations, was successfully applied to the Dobson-based regressions. Additional improvements in the regression algorithm were realized by substituting the radiances in TOVS channel 2 for the radiances in TOVS channel 3. Further improvements were made when the isothermal cases were deleted from the dependent datasets. On an independent set of matched TOVS/Dobson measurements, the ozone derived from the improved set of predictors was more accurate than was the ozone derived from the operational predictors. The standard deviation of the residual errors of the ozone derived from the TOMS-based coefficients was similar to that from the Dobson-based coefficients. The biases were different as would be expected from the well known differences between the Dobson data and the early version of the TOMS data. In the future we will apply these results to a multi-year set of TOVS observations to assess the improvements over different seasons and latitudes.

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